LA-UR-19-26746
Approved for public release; distribution is unlimited.

Title: Modeling Dislocation Dynamics Near Sound Speeds in Cubic Crystals

Author(s): Kleiner, Kevin Gordon
Blaschke, Daniel
Fensin, Saryu Jindal

Intended for: Internal presentation for XCP-5

Issued: 2019-07-23 (rev.1)

Modeling Dislocation Dynamics Near Sound Speeds in Cubic Crystals

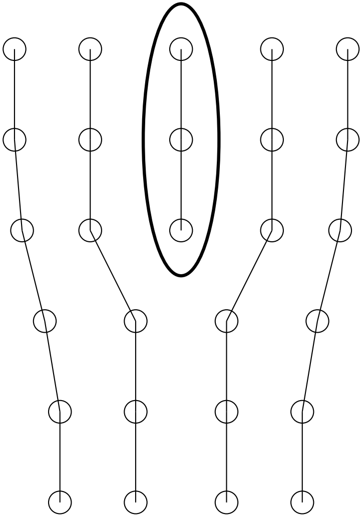
Kevin Gordon Kleiner,
Daniel Blaschke (XCP-5), and
Saryu Fensin (MST-8)

July 22, 2019

Managed by Triad National Security, LLC for the U.S. Department of Energy's NNSA

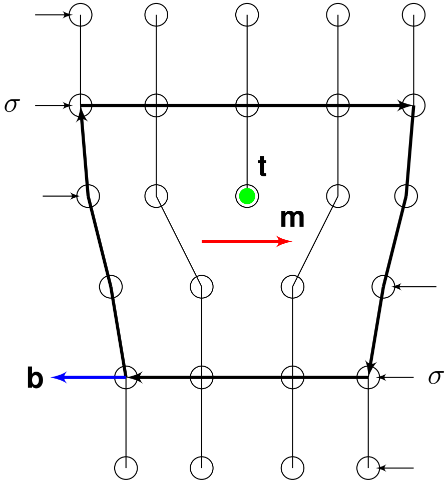
Dislocations as Defects

- Real crystals have many defects that break periodicity
- Curvi-linear defects generated and moved with plastic deformation
- Edge dislocation - extra half-plane between existing planes



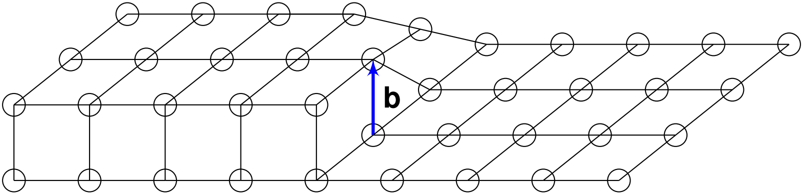
Features of Dislocations

- Circuit discontinuity not in perfect crystals - Burger's vector **b**
- Shear stress σ causes motion **m** in plane spanned by **b** and dislocation line **t**
- Dislocation glide due to breaking and forming bonds near the core



Screw Dislocations

- Winding of atomic planes about an axis
- Vertical jump not in perfect crystals - **b** $\parallel$ **t** point along screw axis[1]
- No single slip plane - crystal geometry dependent
- **b** determined by direction of nearest neighboring atoms



[1] D. Hull and D. J. Bacon, “Defects in Crystals”, in: *Introduction to Dislocations*, 5th ed. Elsevier Ltd., 2011, 1-19.

High Velocity-High Stress Regime

- Little is known about dislocation glide in these conditions
- Possible speed limit by crystal sound waves
- Can dislocations be accelerated past sound speeds without losing stability?
- Material deformation rates strongly related to[2]
  - Mobile dislocation speeds
  - Density of mobile dislocations
  - Time derivative of that density
- Multi-physics simulation codes - build in this high-level data and relevant defect speed limits

[2] P. Rodriguez, *B. Mater. Sci.* **19**, 6 (1996).

Molecular Dynamics (MD) Simulations

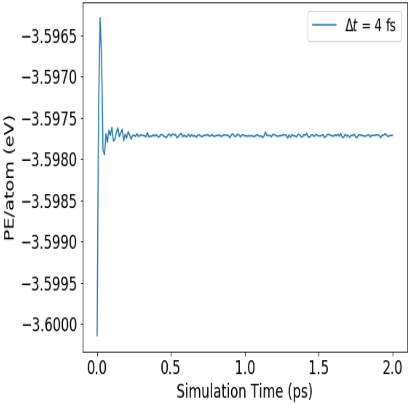
- Individual atoms move around through force evaluations[3]
- Effective forces based on system properties
- Energetically favorable dynamics at femtosecond resolution
- E.g., edge dislocation in face-centered cubic copper splits into partials
- Plastic glide moves both partials simultaneously[4]

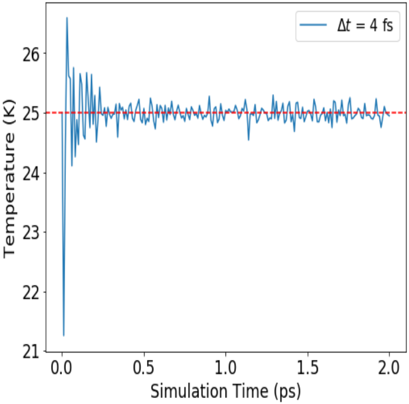
[3] S. Plimpton, *J. Comp. Phys.* **117**, 1-19 (1995).

[4] H. Tsuauki, P. S. Branicio, and J. P. Rino, *Appl. Phys. Lett.* **92**, 191909 (2008).

Copper Initial Equilibration for T = 25 K

- For target temperature, randomly assign atom velocities
- Stabilize configuration accordingly - thermal expansion

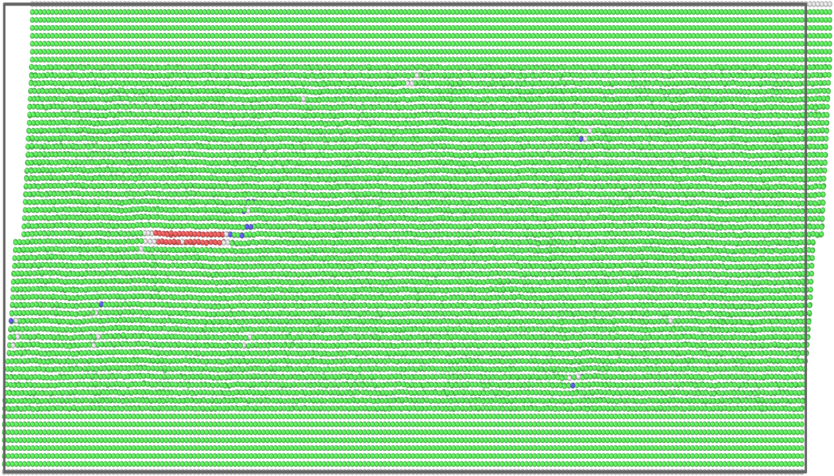




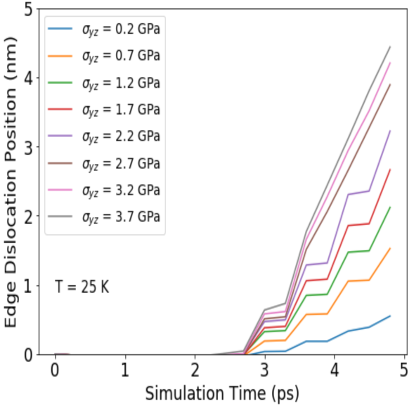
Edge Pair with σ_{yz} = 0.2 GPa at t = 0 ps

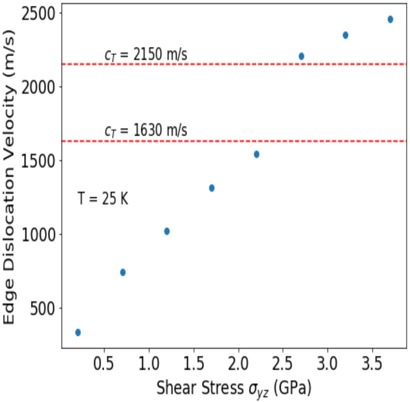
Edge Pair with σ_{yz} = 0.2 GPa at t = 4.2 ps

Edge Pair with σ_{yz} = 0.2 GPa at t = 7.8 ps



Trajectory Dependence on Shear Stress





- Slopes calculated over last 1.8 ps
- Not steady state - velocities smaller than expected in copper

Stress-Strain Relations

- Glide due to plastic deformation, but an elastic model can capture relevant physics

$$\sigma_{ij} = \sum_k \sum_j C_{ijkl} \epsilon_{kl}$$

- Infinitesimal strain ϵ as a gradient of continuum displacement field $\mathbf{u}$

$$\epsilon_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$

- Screw: $\mathbf{u} = (0, 0, u_z(x, y))$ and edge: $\mathbf{u} = (u_x(x, y), u_y(x, y), 0)$ with infinite dislocations lines in z

Introducing Anisotropy

- Cubic symmetry $\Rightarrow$ three independent elastic constants $\{c_{12}, c_{44}, c_{11}\}$ for coordinates aligned with crystal axes - construct stiffness tensor[5]

$$C_{ijkl} = c_{12}\delta_{ij}\delta_{kl} + c_{44}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) - (2c_{44} + c_{12} - c_{11}) \sum_{\alpha} \delta_{i\alpha}\delta_{j\alpha}\delta_{k\alpha}\delta_{l\alpha}$$

- But the simplified components of the dislocation **u** don't align with $\{c_{12}, c_{44}, c_{11}\}$ - rotate the tensor of constants into the slip plane

$$C_{i'j'k'l'} = \sum_{i} \sum_{j} \sum_{k} \sum_{l} R_{i'i} R_{j'j} R_{k'k} R_{l'l} C_{ijkl}$$

[5] D. N. Blaschke and B. A. Szajewski, *Philos. Mag.* **98**, 26 (2018).

Continuum Dislocation Equations of Motion

$$\rho \frac{\partial^2 u_i}{\partial t^2} = \sum_j \frac{\partial \sigma_{ij}}{\partial x_j}$$

- Continuum approximation breaks down at the core $(x, y) = (0, 0)$
- Initial condition:
  - Dislocation stationary at $t = 0$
  - Dislocation accelerating for $t > 0$
- Boundary Conditions:
  - $\mathbf{u}(r_0, \theta_0, z_0, t) = \mathbf{u}(r_0, \theta_0 + 2\pi, z_0, t) + \mathbf{b}$
  - Total stress field balances at dislocation core
- See if strain energy density (1/2)Tr$(\epsilon \cdot \sigma)$ remains finite around the core when accelerating to high speeds

Screw Equation of Motion

- Simplify the tricky coupled system to:

$$\rho \frac{\partial^2 u_z}{\partial t^2} = \frac{\partial \sigma_{xz}}{\partial x} + \frac{\partial \sigma_{yz}}{\partial y} + \frac{\partial \sigma_{zz}}{\partial z}$$

$$\Leftrightarrow A \frac{\partial^2 u_z}{\partial x^2} + B \frac{\partial^2 u_z}{\partial x \partial y} + C \frac{\partial^2 u_z}{\partial y^2} - \rho \frac{\partial^2 u_z}{\partial t^2} = 0$$

- Constants A, B, and C depend on $\{c_{12}, c_{44}, c_{11}\}$ and rotations into the relevant crystal slip plane
- Also impose an acceleration (external stress) as:

$$x = x_0 + \frac{1}{2} a_0 t^2$$

Choice of Initial Condition

- Assume the isotropic static solution is sufficiently close
- $A = C = c_{44}$ and $B = 0$

$$c_{44}\frac{\partial^2 u_z}{\partial x^2} + c_{44}\frac{\partial^2 u_z}{\partial y^2} = 0$$

- The unique solution that satisfies the Burger's circuit condition:[6]

$$u_z(x, y) = \frac{b}{2\pi}\tan^{-1}\left(\frac{y}{x}\right)$$

- Valid outside the dislocation core $(x, y) = (0, 0)$
- Evolve this solution for $t > 0$

[6] J. Weertman, "High Velocity Dislocations", in: *In Response of Metals to High Velocity Deformation*, Ed. P.G. Shewmon and V.F. Zackay. Interscience Publishers, New York, 1961, 205-247.

Numerical Solving Scheme: Finite Difference

- Solve for the screw u_z over time while accelerating
- $x - y$ space replaced by a finite sized discrete mesh
- $u_z(x, y, t) \equiv u^k_{i,j}$
- $u_z(x + \Delta x, y, t) \equiv u^k_{i+1,j}$

$$\frac{\partial^2 u_z}{\partial x^2} = \frac{u^k_{i+1,j} + u^k_{i-1,j} - 2u^k_{i,j}}{\Delta x^2} + \mathcal{O}(\Delta x^2)$$

$$n\Delta x = \frac{1}{2} a_0 t^2_{k+1} - \frac{1}{2} a_0 t^2_k$$

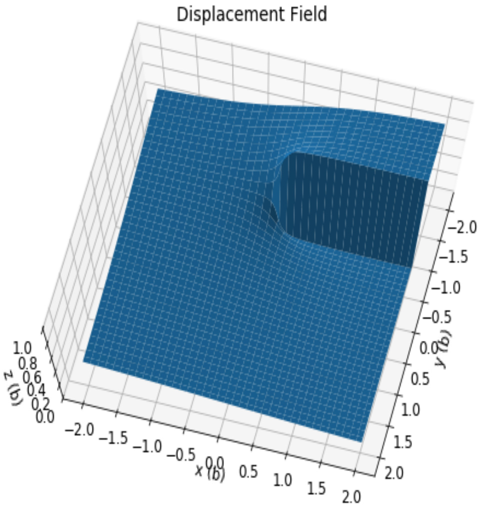
Handling Initial and Boundary Conditions

$$u_{i,j}^{k+1} = \frac{\Delta t^2}{\rho} \left(\frac{A}{\Delta x^2}(u_{i+1,j}^k + u_{i-1,j}^k - 2u_{i,j}^k) + \right.$$
$$\frac{B}{4\Delta x \Delta y}(u_{i+1,j+1}^k - u_{i+1,j-1}^k - u_{i-1,j+1}^k + u_{i-1,j-1}^k)$$
$$\left. + \frac{C}{\Delta y^2}(u_{i,j+1}^k + u_{i,j-1}^k - 2u_{i,j}^k) - \frac{\rho}{\Delta t^2}(u_{i,j}^{k-1} - 2u_{i,j}^k) \right) \tag{1}$$

- When k = 0, the screw is static: $u_{i,j}^{-1} = u_{i,j}^0$
- On boundaries, $u_{i,j}^{k+1} = (b/2\pi)\tan^{-1}(y_j/x_i)$ where y_j accelerates with time

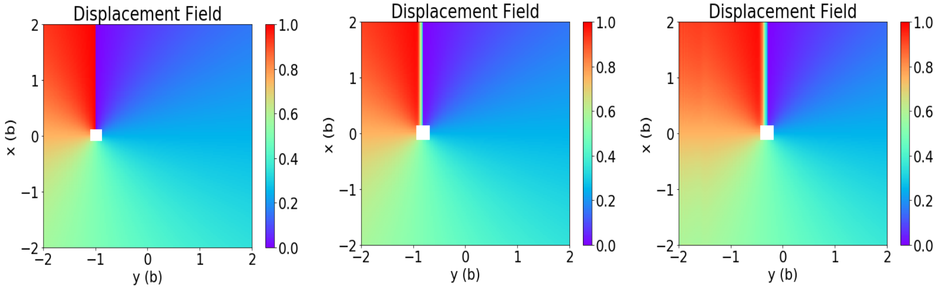
Continuum Screw Dislocation in Aluminum

- Initial form for defect in aluminum: $(b/2\pi)\tan^{-1}(y/x)$
- Models an infinitely winding screw up and down



Aluminum Screw Dislocation Acceleration

- Aluminum has b = 0.286 nm and slowest c_T = 2929 m/s
- Δt = 2.93 fs

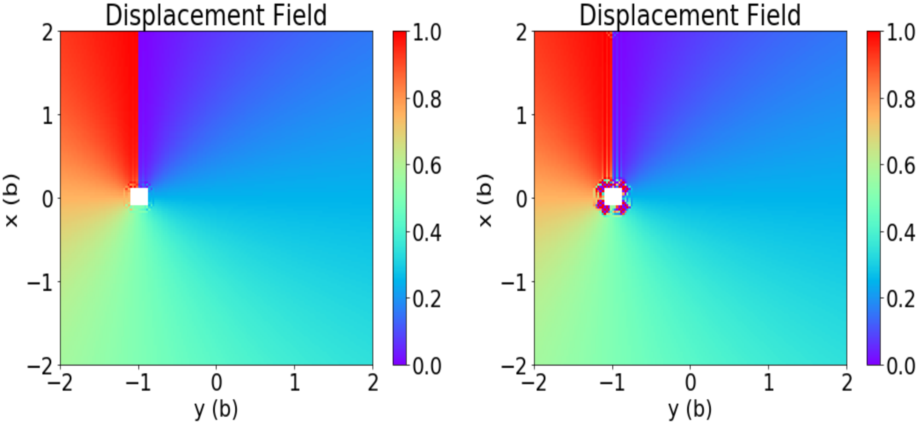


k = 0
v = 0

k = 15
$v = 0.75c_T$

k = 30
$v = 1.50c_T$

Aluminum Screw Dislocation Solver with $a_0 = 0$



$k = 3$ $k = 5$

- Challenge to compute second derivatives near cutout

Conclusions

- MD edge dislocation may outpace transverse sound in copper
  - Wait until steady state for more accuracy
- Continuum equation of motion solving incomplete
  - Numerical instabilities near dislocation core
  - Integrating external acceleration with the solver
  - Start with an anisotropic initial condition
- Possible collaboration opportunity for solving expertise
  - E.g., adaptive mesh refinement to treat the core differently
  - Alternatives schemes - finite elements
- Once successful, different crystal structures/dislocations
- Direct calculations of deformation rates for data in hydro-codes